Mandelic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.11

Global applicability domain: Inside

Local applicability domain index: 3.88e-01

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

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Phenylphosphinic acid
Measured: 6.03
Predicted: 4.42

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2,2-Dimethylpropanoic acid
Measured: 2.29
Predicted: 2.74

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Benzoic acid, 4-(methylamino)-
Measured: 2.40
Predicted: 4.00

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3-Nitrobenzoic acid
Measured: 7.08
Predicted: 3.63

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Sodium 3-nitrobenzenesulfonate
Measured: 5.01
Predicted: 5.24